

A class of piecewise interpolating polynomial approximations for the time-fractional differential equation and its stability analysis

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Abstract

We propose and study a class of numerical schemes to approximate time fractional differential equation. The methods are based on the approximation of the Caputo fractional derivative by piecewise interpolating polynomials, which is strongly related to the backward differentiation formulae for the integer-order case. We investigate their theoretical properties, such as the accuracy and the numerical stability in terms of stability region and $A(\frac{\pi}{2})$ -stability. Numerical experiments are given to verify the theoretical investigations.

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1 Introduction

Fractional calculus, as a generalization of ordinary calculus, has been an intriguing topic for many famous mathematicians since the end of the 17th century. During the last four decades, many scholars have been working on the development of theory for fractional derivatives and integrals, found their way in the world of fractional calculus and their applications. For more detailed information on the historical background, we refer the interested reader to the following books: [38, 41, 37, 39, 25, 26, 6] and [24]. There are several types of fractional derivatives, such as the ones by Caputo, Riemann-Liouville, Riesz and Grünwald-Letnikov (for details on these properties and results, we refer to, e.g., [39]). Differential equations possessing terms with fractional derivatives in the space- or time- or space-time direction have become very important in many application areas. Particularly, in recent years a huge amount of interesting and surprising fractional models have been proposed. Here, we mention just a few typical applications: in the theory of Hankel transforms [17], in financial models [43, 45], in elasticity theory [5, 10], in medical applications [42, 27], in geology [8, 30], in physics [11, 7, 36] and many more.

Similar to the work for ordinary differential equations, that has started more than a century earlier, research on numerical methods for *time-fractional* differential equations (tfDEs) started its development. In this paper we consider approximations to tfDEs in the following form of involving Caputo fractional derivatives of order $0 < \alpha < 1$, i.e.,

$${}^C D^\alpha u(t) = f(t, u(t)), \quad t > 0 \quad (1.1)$$

with initial condition $u(0) = u_0$ and the restriction on given function f for well-posedness of solution [13]. In terms of the numerical approximation of formula (1.1), we mainly concern about the numerical discretisation to the Caputo fractional derivative, the definition of which we refer to Definition 2.1 in the next section. It is observed that the Caputo fractional derivative of a well-behaved function is an operator combined with the integer-order derivative and the fractional integral, which can be regarded as a

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convolution of the weakly singular kernel $t^{-\beta}$ ($0 < \beta < 1$) and a function. The research on numerical approximations to fractional integral was developed in numerically solving a type of Volterra integral equation

$$u(t) = u_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t - \xi)^{\alpha-1} f(\xi, u(\xi)) d\xi, \quad (1.2)$$

which is one of the converting form of (1.1). In terms of numerical approximation to (1.2), a general discrete form can be denoted by

$$u_n = u_0 + (\Delta t)^\alpha \sum_{j=0}^n \omega_{n-j} f(t_j, u_j) + (\Delta t)^\alpha \sum_{j=0}^{k-1} w_{n,j} f(t_j, u_j), \quad n \geq k. \quad (1.3)$$

It deserves to mention the fractional linear multistep methods proposed in [32, 33] in the mid eighties of the last century. This type of methods is devoted to constructing the power series generated by the convolution quadrature weights $\{\omega_j\}_{j=0}^\infty$ based on classical implicit linear multistep formulae (ρ, σ) with the following relationship denoted by

$$\sum_{j=0}^\infty \omega_j \xi^j = \left(\frac{\sigma(1/\xi)}{\rho(1/\xi)} \right)^\alpha,$$

motivation behind which can be referred to [34]. For this type of methods, the accuracy and stability properties are highly benefit from those of corresponding multistep method. Another more straightforward approach to generate the weights $\{\omega_j\}$ and $\{w_{n,j}\}$ is based on quadrature theory applied to the underlying fractional integral, i.e., to replace the integrand $f(\xi, u(\xi))$ by the piecewise Lagrange interpolating polynomials of degree k ($k \geq 0$), and estimate the corresponding fractional integral in (1.2). On the accuracy and efficiency of this class of methods we can refer to [6, 28]. In addition, a series of other approaches were developed. Garappa [21, 20] applies exponential integrators to fractional order problems. Generalized Adams methods and so-called m -steps methods are utilized by Aceto [1, 2]. Other interesting approaches are discussed in the papers [9, 16, 18, 12, 15, 14].

In comparing with previous methods, the numerical approach to solve tfDEs in this paper is arrived at through directly approximating fractional derivative combining with numerical differentiation and integration. Recently, a new type of numerical schemes was designed to approximate the Caputo fractional derivative for solving time fractional partial differential equations, such as $L1$ method [29], $L1-2$ method [19], $L2-1_\sigma$ method [4]. These methods are all based on piecewise linear or quadratic interpolating polynomials approximation. It is natural to generalise the approach by improving the degree of the piecewise polynomial to approximate function that possesses suitable smoothness, in which situation the higher order of accuracy can be obtained. In the next section, we will devote to deriving a series of numerical schemes for formula (1.1) based on constructing piecewise interpolation polynomials on interval $[0, t]$ as the approximations to solution $u(t)$, and consequently, the α order Caputo derivative of the polynomials as the approximation to ${}^C D^\alpha u(t)$. The local truncation errors of the numerical schemes are discussed correspondingly. The flexibility via choosing different interpolating points on subintervals to construct the piecewise polynomials will produce various schemes under the similar restriction of accuracy order.

In order to study the numerical stability of such methods applying to problem (1.1), we will examine the behaviour of the numerical method on the linear scalar equation

$${}^C D^\alpha u(t) = \lambda u(t), \quad \lambda \in \mathbb{C} \quad (1.4)$$

with initial value $u(0) = u_0$. It is already shown that the solution of (1.4) satisfies that $u(t) \rightarrow 0$ as $t \rightarrow +\infty$ provided that $|\arg(\lambda)| > \frac{\alpha\pi}{2}$ ($-\pi \leq \arg(\lambda) \leq \pi$) for arbitrary bounded initial value [33, 35], accordingly, it can be studied in seeking those λ for which the corresponding numerical solutions preserve the same property as true solution. In fact, several classical numerical stability theories have been constructed on solving problem (1.4) in the case of $\alpha = 1$ [22, 23]. Furthermore, there are some efforts on generalising the numerical stability theory on linear multistep methods to integral equations, such as Volterra-type integral equation [31, 33]. It is known that, for example, in the case of all those λ satisfying $|\arg(\lambda)| > \frac{\alpha\pi}{2}$ ($0 < \alpha \leq 1$), if the numerical solution has the same asymptotical stability property as true solution, the numerical method is called A -stable, and in other case of λ falling into the sector with $|\arg(\lambda)| \geq \theta$ ($\frac{\alpha\pi}{2} < |\theta| \leq \pi$), it is referred to as $A(\theta)$ -stable. Inspired by the previous work, in this paper, we confirm

the stability regions of the proposed numerical methods and provide the rigorous analysis on the $A(\frac{\pi}{2})$ -stability of some methods. Actually, it can be observed from the numerical experiments that the class of methods possesses the $A(\theta)$ -stability property rather than the A -stability uniformly for $0 < \alpha < 1$.

The paper is organized as follows. Section 2 introduces the piecewise interpolation approximations of the Caputo derivative. Here, we also derive some useful properties of the weight coefficients and discuss the truncation errors. Section 3 treats the stability aspects of the numerical schemes when applied to time-fractional differential equations. In section 4 numerical experiments confirm our theoretical considerations with respect to order of convergence and stability restrictions.

2 Piecewise interpolating polynomial approximation to the Caputo fractional derivative

The fractional derivative in the Caputo sense is introduced as follows:

Definition 2.1 ([13]). *Let $\alpha > 0$, and $n = \lceil \alpha \rceil$, the α order Caputo derivative of function $u(t)$ on $[0, T]$ is defined by*

$${}^C D^\alpha u(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{u^{(n)}(\xi)}{(t-\xi)^{\alpha-n+1}} d\xi \quad (2.1)$$

whenever $u^{(n)}(t) \in L_1[0, T]$. In particular, the Caputo derivative of order $\alpha \in (0, 1)$ is defined by

$${}^C D^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\xi)^{-\alpha} u^{(1)}(\xi) d\xi \quad (2.2)$$

whenever $u^{(1)}(t) \in L_1[0, T]$.

In this section we concentrate on deriving piecewise interpolating polynomial approximations to the Caputo fractional derivative of order $\alpha \in (0, 1)$, and in principle, the main ideas can be extended to arbitrary order fractional derivatives $\alpha > 0$ as well.

A uniform partition of interval $[0, T]$ is given by

$$0 = t_0 < t_1 < \dots < t_{M-1} < t_M = T,$$

where $t_n = n\Delta t$ and $\Delta t = \frac{T}{M}$ as $M \in \mathbb{N}^+$. The piecewise function $p_{j,q}^k(t)$ is expressed by the interpolating polynomial of degree k over the subinterval $[t_{j-1}, t_j]$, i.e.,

$$p_{j,q}^k(t) = p_{j,q}^k(t_{j-1} + s\Delta t) = \sum_{r=0}^k \binom{s-q+r-1}{r} \nabla^r u(t_{j+q-1}), \quad q \in \mathbb{N}^+ \quad (2.3)$$

and vanishes otherwise, where the r -th order backward difference operator ∇^r is defined by

$$\nabla^0 u(t_i) = u(t_i), \quad \nabla^r u(t_i) = \nabla^{r-1} u(t_i) - \nabla^{r-1} u(t_{i-1})$$

and $\binom{s-q+r-1}{r}$ is the binomial coefficient. Thus, according to (2.3), it is satisfied that

$$p_{j,q}^k(t_i) = u(t_i), \quad i = j-1, j \quad (2.4)$$

in the case of $q, k \in \mathbb{N}^+$ and $q \leq k$.

In the following, a class of piecewise continuous polynomials $P_i^k(t)$ ($1 \leq i \leq k \leq 6$) are constructed on $t \in [0, \tau]$ for $\tau \in (t_{n-1}, t_n]$ and $n \geq k$ with the following form

$$P_i^k(t) = \sum_{j=1}^{k-i} p_{j,k-j}^{k-1}(t) + \sum_{j=k}^n p_{j-i+1,i}^k(t) + \sum_{j=n-i+2}^n p_{j,n+1-j}^k(t),$$

in combination with the definitions of $\sum_{j=1}^{k-i} p_{j,k-j}^{k-1}(t) = 0$ and $\sum_{j=n-i+2}^n p_{j,n+1-j}^k(t) = 0$ for $k-i < 1$ and $n-i+2 > n$, respectively. As a consequence, the following difference operator

$$D_{k,i}^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\xi)^{-\alpha} \frac{dP_i^k}{d\xi} d\xi \quad (2.5)$$

is given on $t \in (t_{n-1}, t_n]$ for $n \geq k$. In the case of $t = t_n$, formula (2.5) can also be rewritten to

$$D_{k,i}^\alpha u_n = (\Delta t)^{-\alpha} \sum_{j=0}^{k-1} w_{n,j}^{(k,i)} u_j + (\Delta t)^{-\alpha} \sum_{j=0}^n \omega_{n-j}^{(k,i)} u_j, \quad (2.6)$$

where $u_n := u(t_n)$.

In the following text, we will compare with the weight coefficients $\{w_{n,j}^{(k,i)}\}$ and $\{\omega_j^{(k,i)}\}$ for $1 \leq i \leq k \leq 3$ as examples. First, we define that

$$I_{n,q}^r = \begin{cases} \frac{1}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha} d\left(\frac{s^{-q+r-1}}{r}\right), & n \geq 0, \\ 0, & n < 0, \end{cases} \quad (2.7)$$

where $q, r \in \mathbb{N}^+$ and $n \in \mathbb{Z}$. In addition, denote that

$$\begin{aligned} I_n &:= I_{n,q}^1, \quad \forall q = 1, 2, \dots, \\ \nabla^k I_{n,q}^r &= \nabla^{k-1} I_{n,q}^r - \nabla^{k-1} I_{n-1,q}^r, \quad \forall k \in \mathbb{N}^+. \end{aligned}$$

Then we can derive the following expressions

$$\begin{cases} (k,i) = (1,1): w_{m,0} = -I_m, \quad m \geq 1, \quad \omega_n = \nabla I_n, \quad n \geq 0, \\ (k,i) = (2,1): w_{m,0} = 2I_{m-1,1}^2 - I_{m,1}^2 - I_m, \quad w_{m,1} = -I_{m-1,1}^2, \quad m \geq 2, \\ \quad \omega_n = \nabla I_n + \nabla^2 I_{n,1}^2, \quad n \geq 0, \\ (k,i) = (2,2): w_{m,0} = -\nabla I_{m+1,1}^2 + I_{m,2}^2, \quad w_{m,1} = -I_{m,1}^2, \quad m \geq 2, \\ \quad \omega_0 = I_0 + I_1 + I_{0,1}^2 + I_{1,2}^2, \quad \omega_1 = \nabla I_2 - I_0 + I_{2,2}^2 - 2I_{0,1}^2 - 2I_{1,2}^2, \\ \quad \omega_2 = \nabla I_3 + \nabla^2 I_{3,2}^2 + I_{0,1}^2, \quad \omega_n = \nabla I_{n+1} + \nabla^2 I_{n+1,2}^2, \quad n \geq 3, \end{cases}$$

and more complicated formulae with

(1). $(k,i) = (3,1)$,

$$\begin{cases} w_{m,0} = -\nabla I_m - I_{m,1}^2 + 2I_{m-1,1}^2 + I_{m-1,2}^2 - I_{m,1}^3 + 3I_{m-1,1}^3 - 3I_{m-2,1}^3, \\ w_{m,1} = -2I_{m-1} - 2I_{m-1,2}^2 - I_{m-1,1}^2 - I_{m-1,1}^3 + 3I_{m-2,1}^3, \\ w_{m,2} = I_{m-1} + I_{m-1,2}^2 - I_{m-2,1}^3, \quad m \geq 3, \\ \omega_n = \nabla I_n + \nabla^2 I_{n,1}^2 + \nabla^3 I_{n,1}^3, \quad n \geq 0, \end{cases}$$

(2). $(k,i) = (3,2)$,

$$\begin{cases} w_{m,0} = -\nabla I_{m+1} - I_{m+1,2}^2 + 2I_{m,2}^2 - I_{m+1,2}^3 + 3I_{m,2}^3 - 3I_{m-1,2}^3, \\ w_{m,1} = -I_m - I_{m,2}^2 - I_{m,2}^3 + 3I_{m-1,2}^3, \\ w_{m,2} = -I_{m-1,2}^3, \quad m \geq 3, \\ \omega_0 = I_0 + I_1 + I_{1,2}^2 + I_{0,1}^2 + I_{1,2}^3 + I_{0,1}^3, \\ \omega_1 = \nabla I_2 - I_0 + I_{2,2}^2 - 2I_{1,2}^2 - 2I_{0,1}^2 + I_{2,2}^3 - 3I_{1,2}^3 - 3I_{0,1}^3, \\ \omega_2 = \nabla I_3 + \nabla^2 I_{3,2}^2 + I_{0,1}^2 + I_{3,2}^3 - 3I_{2,2}^3 + 3I_{1,2}^3 + 3I_{0,1}^3, \\ \omega_3 = \nabla I_4 + \nabla^2 I_{4,2}^2 + \nabla^3 I_{4,2}^3 - I_{0,1}^3, \\ \omega_n = \nabla I_{n+1} + \nabla^2 I_{n+1,2}^2 + \nabla^3 I_{n+1,2}^3, \quad n \geq 4, \end{cases}$$

(3). $(k, i) = (3, 3)$,

$$\begin{cases} w_{m,0} = -\nabla I_{m+2} - \nabla^2 I_{m+2,3}^2 - I_{m+2,3}^3 + 3I_{m+1,3}^3 - 3I_{m,3}^3, \\ w_{m,1} = -\nabla I_{m+1} - I_{m+1,3}^2 + 2I_{m,3}^2 - I_{m+1,3}^3 + 3I_{m,3}^3, \\ w_{m,2} = -I_m - I_{m,3}^2 - I_{m,3}^3, \quad m \geq 3, \\ \omega_0 = I_0 + I_1 + I_2 + I_{0,1}^2 + I_{1,2}^2 + I_{2,3}^2 + I_{0,1}^3 + I_{1,2}^3 + I_{2,3}^3, \\ \omega_1 = \nabla I_3 - I_0 - I_1 + I_{3,3}^2 - 2I_{2,3}^2 - 2I_{1,2}^2 - 2I_{0,1}^2 + I_{3,3}^3 - 3I_{2,3}^3 - 3I_{1,2}^3 - 3I_{0,1}^3, \\ \omega_2 = \nabla I_4 + \nabla^2 I_{4,3}^2 + I_{1,2}^2 + I_{0,1}^2 + I_{4,3}^3 - 3I_{3,3}^3 + 3I_{2,3}^3 + 3I_{0,1}^3 + 3I_{1,2}^3, \\ \omega_3 = \nabla I_5 + \nabla^2 I_{5,3}^2 + \nabla^3 I_{5,3}^3 - I_{1,2}^3 - I_{0,1}^3, \\ \omega_n = \nabla I_{n+2} + \nabla^2 I_{n+2,3}^2 + \nabla^3 I_{n+2,3}^3, \quad n \geq 4. \end{cases}$$

Observe that for $\alpha \rightarrow 1$, the difference operator $D_{k,i}^\alpha u_n$ in (2.6) recover to the k -step BDFs.

2.1 Complete monotonicity and error analysis

In the following, we explore the completely monotonic property of sequence $\{I_{n,q}^r\}_{n=0}^\infty$.

Lemma 2.1. Assume that $I_{n,q}^r$ is defined by (2.7), then for $n \geq k$ with $k \in \mathbb{N}$, it holds that

$$(-1)^{k+r+1} \nabla^k I_{n,q}^r \geq 0 \quad (2.8)$$

in the case of $r \leq q$, and

$$(-1)^{k+q+1} \nabla^k I_{n,q}^r \geq 0 \quad (2.9)$$

in the case of $r > q$.

Proof. We begin with the case of $r \leq q$, according to the definition of $I_{n,q}^r$ in (2.7), it holds that

$$\begin{aligned} I_{n,q}^r &= \frac{1}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha} d \binom{s-q+r-1}{r} \\ &= \frac{1}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha} \sum_{n=0}^{r-1} \frac{1}{(s-q+n)} \binom{s-q+r-1}{r} ds, \end{aligned}$$

since $(s-q+n) \leq 0$ for $0 \leq s \leq 1$ and $n = 0, \dots, r-1$, it yields that $(-1)^r \binom{s-q+r-1}{r} \geq 0$, and consequently $(-1)^{r+1} \frac{d}{ds} \binom{s-q+r-1}{r} \geq 0$, combined with $(n+1-s)^{-\alpha} > 0$ for any $n \geq 0$ and $\alpha > 0$, it leads to $(-1)^{r+1} I_{n,q}^r \geq 0$. In addition, by definition, we may see that

$$\begin{aligned} \nabla I_{n,q}^r &= \frac{1}{\Gamma(1-\alpha)} \int_0^1 \left((n+1-s)^{-\alpha} - (n-s)^{-\alpha} \right) d \binom{s-q+r-1}{r} \\ &= \frac{-\alpha}{\Gamma(1-\alpha)} \int_0^1 \int_n^{n+1} (\xi-s)^{-\alpha-1} d\xi d \binom{s-q+r-1}{r} \\ &= \frac{-\alpha}{\Gamma(1-\alpha)} \int_0^1 \int_0^1 (\xi+n-s)^{-\alpha-1} d\xi d \binom{s-q+r-1}{r}, \end{aligned}$$

with $(\xi+n-s)^{-\alpha-1} \geq 0$ for $n \geq 1$ and $0 \leq \xi, s \leq 1$, then $(-1)^{r+2} \nabla I_{n,q}^r \geq 0$.

Assume that for $k \geq 2$, it holds

$$\nabla^{k-1} I_{n,q}^r = \frac{(-\alpha)_{k-1}}{\Gamma(1-\alpha)} \int_{[0,1]^k} \left(\sum_{i=1}^{k-1} \xi_i + n - k + 2 - s \right)^{-\alpha-k+1} d^{k-1} \xi d \binom{s-q+r-1}{r},$$

where $(\alpha)_{k-1} = \alpha(\alpha-1)\cdots(\alpha-k+2)$ and $d^{k-1}\xi = d\xi_1 \cdots d\xi_{k-1}$, then

$$\begin{aligned} \nabla^k I_{n,q}^r &= \nabla^{k-1} I_{n,q}^r - \nabla^{k-1} I_{n-1,q}^r \\ &= \frac{(-\alpha)_{k-1}}{\Gamma(1-\alpha)} \int_{[0,1]^k} \nabla \left(\sum_{i=1}^{k-1} \xi_i + n - k + 2 - s \right)^{-\alpha-k+1} d^{k-1}\xi d \binom{s-q+r-1}{r} \\ &= \frac{(-\alpha)_k}{\Gamma(1-\alpha)} \int_{[0,1]^k} \int_{n+1}^{n+2} \left(\sum_{i=1}^k \xi_i - k - s \right)^{-\alpha-k} d\xi_k d^{k-1}\xi d \binom{s-q+r-1}{r} \\ &= \frac{(-\alpha)_k}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} \left(\sum_{i=1}^k \xi_i + n - k + 1 - s \right)^{-\alpha-k} d^k \xi d \binom{s-q+r-1}{r}. \end{aligned}$$

Since $(\sum_{i=1}^k \xi_i + n - k + 1 - s) \geq 0$ for $n \geq k \geq 1$ and $0 \leq \xi_i, s \leq 1$, (2.8) holds.

In the other case of $r \geq q+1$, integrating by part yields that

$$\begin{aligned} I_{n,q}^r &= \frac{1}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha} d \binom{s-q+r-1}{r} \\ &= \frac{-\alpha}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha-1} \binom{s-q+r-1}{r} ds, \end{aligned}$$

since $\binom{s-q+r-1}{r}$ includes factor $s(s-1)$ for $r \geq q+1, q \in \mathbb{N}^+$. The sign of $\binom{s-q+r-1}{r}$ is the same with that of $\prod_{i=1}^q (s-i)$, thus there is $(-1)^q \binom{s-q+r-1}{r} \geq 0$, and it holds that $(-1)^{q+1} I_{n,q}^r \geq 0$ for $n \geq 0$. Furthermore, the induction process demonstrates that

$$\nabla^k I_{n,q}^r = \frac{(-\alpha)_{k+1}}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} \left(\sum_{i=1}^k \xi_i + n - k + 1 - s \right)^{-\alpha-k-1} \binom{s-q+r-1}{r} d^k \xi ds$$

for $n \geq k \geq 1$, which arrives at (2.9). \square

If applying (2.6) to numerically solve problem (1.1) with

$$D_{k,i}^\alpha u_n = f(t_n), \quad n \geq k, \quad (2.10)$$

the truncation error of the n -th step is defined by

$$\tau_n^{(k,i)} = D_{k,i}^\alpha u(t_n) - {}^C D^\alpha u(t_n), \quad n \geq k, \quad n \in \mathbb{N}^+, \quad (2.11)$$

where $u(t)$ is the exact solution of problem (1.1).

Theorem 2.1. Assume that $u \in C^{k+1}[0, T]$ and $0 < \alpha < 1$, it holds that

$$D_{k,i}^\alpha u(t_n) - {}^C D^\alpha u(t_n) = O \left((t_{n-k+i})^{-\alpha-1} \Delta t^{k+1} + \Delta t^{k+1-\alpha} \right),$$

for $n \geq k$ in the cases of $1 \leq i < k \leq 6$. In particular

$$D_{k,k}^\alpha u(t_n) - {}^C D^\alpha u(t_n) = O(\Delta t^{k+1-\alpha}), \quad k = 1, \dots, 6$$

holds uniformly for $n \geq k$.

Proof. According to (2.3), it holds that

$$p_{j,q}^k(t) - u(t) = u^{(k+1)}(\xi_j) \binom{s-q+k}{k+1} (\Delta t)^{k+1}, \quad (2.12)$$

where $t = t_{j-1} + s\Delta t$ with $0 \leq s \leq 1$ and $t_{j+q-k-1} \leq \xi_j \leq t_{j+q-1}$.

Inspired by [19], making use of the integration by part technique, we arrive at

$$\begin{aligned} D_{k,i}^\alpha u(t_n) - {}^C D^\alpha u(t_n) &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^n \int_{t_{j-1}}^{t_j} (t_n - t)^{-\alpha} \left(\frac{dP_i^k}{dt} - \frac{du}{dt} \right) dt \\ &= \frac{-\alpha}{\Gamma(1-\alpha)} \sum_{j=1}^n \int_{t_{j-1}}^{t_j} (t_n - t)^{-\alpha-1} (P_i^k - u) dt \end{aligned}$$

for $n \geq k$, which is based on the conditions of (2.4) and (2.12). Therefore, it holds that

$$D_{k,i}^\alpha u(t_n) - {}^C D^\alpha u(t_n) = \frac{-\alpha(\Delta t)^{k+1-\alpha}}{\Gamma(1-\alpha)} \sum_{j=1}^n \int_0^1 (n-j+1-s)^{-\alpha-1} (P_i^k(t_{j-1} + s\Delta t) - u(t_{j-1} + s\Delta t)) ds. \quad (2.13)$$

Since for any $q \leq k$ and $q, k \in \mathbb{N}^+$, the factor $(1-s)$ is included in $\binom{s-q+k}{k+1}$ and $\frac{1}{1-s} \binom{s-q+k}{k+1}$ is bounded for $0 \leq s \leq 1$, thus we can obtain that

$$\begin{aligned} |D_{k,i}^\alpha u(t_n) - {}^C D^\alpha u(t_n)| &\leq \frac{\alpha(\Delta t)^{k+1-\alpha}}{\Gamma(1-\alpha)} C^{(k)} \sum_{j=1}^n \int_0^1 (n-j+1-s)^{-\alpha-1} (1-s) ds \\ &\leq \frac{\alpha(\Delta t)^{k+1-\alpha}}{\Gamma(1-\alpha)} C^{(k)} \left(\sum_{j=1}^{n-1} \int_0^1 (n-j+1-s)^{-\alpha-1} ds + \int_0^1 (1-s)^{-\alpha} ds \right) \\ &\leq (\Delta t)^{k+1-\alpha} C^{(k)} \left(\frac{1}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(2-\alpha)} \right), \end{aligned}$$

where $C^{(k)}$ is bounded relevant to $u^{(k+1)}$ and k . Moreover, the definition of P_i^k for $i < k$ and (2.13) yield that

$$\begin{aligned} |D_{k,i}^\alpha u(t_n) - {}^C D^\alpha u(t_n)| &\leq \frac{\alpha}{\Gamma(1-\alpha)} C^{(k,i)} \left((\Delta t)^{k-\alpha} \sum_{j=1}^{k-i} \int_0^1 (n-j+1-s)^{-\alpha-1} ds \right. \\ &\quad \left. + (\Delta t)^{k+1-\alpha} \sum_{j=1}^n \int_0^1 (n-j+1-s)^{-\alpha-1} (1-s) ds \right) \\ &\leq C^{(k,i)} \left(\frac{\alpha}{\Gamma(1-\alpha)} (\Delta t)^{k+1} (k-i)(t_{n-k+i})^{-\alpha-1} \right. \\ &\quad \left. + (\Delta t)^{k+1-\alpha} \left(\frac{1}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(2-\alpha)} \right) \right), \end{aligned}$$

where $C^{(k,i)}$ is a constant depending on $u^{(k)}$, $u^{(k+1)}$ and k, i . □

3 Stability analysis

To consider the numerical stability of schemes (2.10) with initial value $u(0) = u_0$, the analyses on the linear difference equation

$$D_{k,i}^\alpha u_n = \lambda u_n, \quad n \geq k, \quad (3.1)$$

or equivalently,

$$\omega^{(k,i)}(\xi) u(\xi) = z u(\xi) + g^{(k,i)}(\xi), \quad z := \lambda(\Delta t)^\alpha \quad (3.2)$$

is given as follows, where the formal power series are

$$\begin{aligned} u(\xi) &= \sum_{n=0}^{\infty} u_{n+k} \xi^n, \quad \omega^{(k,i)}(\xi) = \sum_{n=0}^{\infty} \omega_n^{(k,i)} \xi^n, \\ g^{(k,i)}(\xi) &= - \sum_{j=0}^{k-1} u_j \sum_{n=0}^{\infty} (w_{n+k,j}^{(k,i)} + \omega_{n+k-j}^{(k,i)}) \xi^n. \end{aligned} \quad (3.3)$$

Inspired by [31, 33], we list the following preliminary conclusions.

Lemma 3.1 ([33]). Assume that the coefficient sequence of $a(\xi)$ is in l^1 . Let $|\xi_0| \leq 1$. Then the coefficient sequence of

$$b(\xi) = \frac{a(\xi) - a(\xi_0)}{\xi - \xi_0}$$

converges to zero.

Theorem 3.1 ([40, 46]). Suppose that

$$f(z) = \sum_{n=0}^{\infty} c_n z^n, \quad \sum_{n=0}^{\infty} |c_n| < \infty,$$

and $f(z) \neq 0$ for every $|z| \leq 1$. Then

$$\frac{1}{f(z)} = \sum_{n=0}^{\infty} a_n z^n \quad \text{with} \quad \sum_{n=0}^{\infty} |a_n| < \infty.$$

Theorem 3.2 ([3, 44]). For the moment problem

$$s_k = \int_0^1 u^k d\sigma(u), \quad k = 0, 1, \dots$$

to be soluble within the class of non-decreasing functions iff the inequalities

$$(-1)^m \nabla^m s_k \geq 0$$

hold for $k \geq m$.

Lemma 3.2. The coefficient sequences of series $g^{(k,i)}(\xi)$ converge to zero.

Proof. According to the expression of $\nabla^k I_{n,q}^r$ in Lemma 2.1, it yields that

$$\lim_{n \rightarrow \infty} \nabla^k I_{n,q}^r = \frac{(-\alpha)_k}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} \lim_{n \rightarrow \infty} \left(\sum_{i=1}^k \xi_i + n - k + 1 - s \right)^{-\alpha-k} d^k \xi d \binom{s-q+r-1}{r} = 0$$

or

$$\lim_{n \rightarrow \infty} \nabla^k I_{n,q}^r = \frac{(-\alpha)_{k+1}}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} \lim_{n \rightarrow \infty} \left(\sum_{i=1}^k \xi_i + n - k + 1 - s \right)^{-\alpha-k-1} \binom{s-q+r-1}{r} d^k \xi ds = 0$$

for $k, q, r \in \mathbb{N}^+$ that are independent of n and $\alpha > 0$. Note that $g_n^{(k,i)} = -\sum_{j=0}^{k-1} u_j (w_{n+k,j}^{(k,i)} + \omega_{n+k-j}^{(k,i)})$ is

the finite linear combination of $\nabla^k I_{j,q}^r$ for finite k , thus it deduces $g_n^{(k,i)} \rightarrow 0$ as $n \rightarrow \infty$ if $\{u_j\}_{j=0}^{k-1}$ are bounded. \square

Lemma 3.3. For $1 \leq i \leq k \leq 6$, the coefficient sequence of $\omega^{(k,i)}(\xi)$ belongs to l^1 space.

Proof. As indicated in Lemma 2.1 and Lemma 3.2, the following relationship

$$\sum_{n=p}^{\infty} |\nabla^k I_{n,q}^r| = \left| \sum_{n=p}^{\infty} (\nabla^{k-1} I_{n,q}^r - \nabla^{k-1} I_{n-1,q}^r) \right| = |\nabla^{k-1} I_{p-1,q}^r| \quad (3.4)$$

holds for $p \geq k \geq 1$. Therefore, according to the definition of sequence $\{\omega_n^{(k,i)}\}_{n=0}^{\infty}$, there exists finite positive integer $M = M(k, i)$, such that

$$\begin{aligned} \sum_{n=0}^{\infty} |\omega_n^{(k,i)}| &\leq \sum_{n=0}^M |\omega_n^{(k,i)}| + \sum_{m=1}^k \sum_{n=m}^{\infty} |\nabla^m I_{n,i}^m| \\ &\leq \sum_{n=0}^M |\omega_n^{(k,i)}| + \sum_{m=1}^k |\nabla^{m-1} I_{m-1,i}^m|, \end{aligned}$$

which implies the result. \square

Lemma 3.4. For $1 \leq i \leq k \leq 6$ and $|\xi_0| \leq 1$, the coefficient sequence of $(1 - \xi) \frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0}$ belongs to l^1 sapce.

Proof. According to the expression of $\omega^{(k,i)}(\xi)$, the following series can be rewritten to

$$\begin{aligned} (1 - \xi) \frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0} &= (1 - \xi) \sum_{n=0}^{\infty} \omega_n^{(k,i)} \frac{\xi^n - \xi_0^n}{\xi - \xi_0} \\ &= (1 - \xi) \sum_{n=1}^{\infty} \omega_n^{(k,i)} \sum_{m=0}^{n-1} \xi_0^{n-1-m} \xi^m \\ &= (1 - \xi) \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \omega_{n+m+1}^{(k,i)} \xi_0^n \xi^m \\ &= \sum_{n=0}^{\infty} \omega_{n+1}^{(k,i)} \xi_0^n + \sum_{m=1}^{\infty} \left(\sum_{n=0}^{\infty} \nabla \omega_{n+m+1}^{(k,i)} \xi_0^n \right) \xi^m. \end{aligned}$$

On one hand, from Lemma 3.3, we have

$$\left| \sum_{n=0}^{\infty} \omega_{n+1}^{(k,i)} \xi_0^n \right| \leq \sum_{n=0}^{\infty} |\omega_{n+1}^{(k,i)}| |\xi_0|^n \leq \sum_{n=0}^{\infty} |\omega_{n+1}^{(k,i)}| < +\infty.$$

On the other hand, by the definition of $\{\nabla^{k+1} I_{n,q}^r\}_{n=k+1}^{\infty}$ in Lemma 2.1, it can be verified that

$$\begin{aligned} \sum_{m=p}^{\infty} \sum_{n=0}^{\infty} |\nabla^{k+1} I_{m+n+1,q}^r| &= \left| \sum_{m=p}^{\infty} \sum_{n=0}^{\infty} (\nabla^k I_{m+n+1,q}^r - \nabla^k I_{m+n,q}^r) \right| \\ &= \left| \sum_{m=p}^{\infty} (\nabla^{k-1} I_{m,q}^r - \nabla^{k-1} I_{m-1,q}^r) \right| \\ &= |\nabla^{k-1} I_{p-1,q}^r| \end{aligned}$$

for $p \geq k \geq 1$. Therefore there exists $M_1 = M_1(k, i) \geq 1$ and $M_2 = M_2(k, i) \geq 0$ such that

$$\begin{aligned} \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} |\nabla \omega_{n+m+1}^{(k,i)}| &\leq \sum_{m=1}^{M_1} \sum_{n=0}^{M_2} |\nabla \omega_{n+m+1}^{(k,i)}| + \sum_{p=1}^k \sum_{m=p}^{\infty} \sum_{n=0}^{\infty} |\nabla^{p+1} I_{m+n+1,i}^p| \\ &\leq \sum_{m=1}^{M_1} \sum_{n=0}^{M_2} |\nabla \omega_{n+m+1}^{(k,i)}| + \sum_{p=1}^k |\nabla^{p-1} I_{p-1,i}^p|. \end{aligned}$$

Combining with

$$\left| \sum_{n=0}^{\infty} \omega_{n+1}^{(k,i)} \xi_0^n \right| + \sum_{m=1}^{\infty} \left| \sum_{n=0}^{\infty} \nabla \omega_{n+m+1}^{(k,i)} \xi_0^n \right| \leq \sum_{n=0}^{\infty} |\omega_{n+1}^{(k,i)}| + \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} |\nabla \omega_{n+m+1}^{(k,i)}|,$$

we arrive at the conclusion. \square

Theorem 3.3. The stability region of method $D_{k,i}^\alpha u_n = \lambda u_n$ is $S^{(k,i)} = \mathbb{C} \setminus \{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$ in the cases of $1 \leq i \leq k \leq 6$.

Remark 1. The definition of stability region $S^{(k,i)}$ of method $D_{k,i}^\alpha u_n = \lambda u_n$ is the set of $z \in \mathbb{C}$ with $\Delta t > 0$ for which there is $u_n \rightarrow 0$ as $n \rightarrow \infty$ whenever the starting values u_0, \dots, u_{k-1} are bounded.

Proof. The provement of $S^{(k,i)} = \mathbb{C} \setminus \{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$ is equivalent with proving both $S^{(k,i)} \supseteq \mathbb{C} \setminus \{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$ and $S^{(k,i)} \subseteq \mathbb{C} \setminus \{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$, i.e., to prove that for any $z \in \mathbb{C} \setminus \{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$, there is $z \in S^{(k,i)}$ and for any $z \notin \mathbb{C} \setminus \{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$, there is $z \notin S^{(k,i)}$.

On one hand, if $z \in \mathbb{C} \setminus \{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$ and $|z| \leq 1$, there is $z - \omega^{(k,i)}(\xi) \neq 0$ for $|\xi| \leq 1$, thus according to Lemma 3.2, Lemma 3.3 and Theorem 3.1, it yields that the coefficient sequence of reciprocal of $z - \omega^{(k,i)}(\xi)$ is in l^1 and coefficient sequence of series $g^{(k,i)}(\xi)$ tends to zero.

If $|z| > 1$, formula (3.2) can be rewritten to

$$u(\xi) = \frac{\frac{g^{(k,i)}(\xi)}{z}}{\frac{\omega^{(k,i)}(\xi)}{z} - 1},$$

in which case the coefficient sequence of reciprocal of $\frac{\omega^{(k,i)}(\xi)}{z} - 1$ is in l^1 , and the coefficient sequence of series $\frac{g^{(k,i)}(\xi)}{z}$ converges to zero. In addition, assume that $\lim_{n \rightarrow \infty} \sum_{j=0}^n |l_j| = L < \infty$ and $\lim_{j \rightarrow \infty} c_j = 0$, it holds that $\lim_{n \rightarrow \infty} \sum_{j=0}^n l_{n-j} c_j = 0$, thus, it implies that $u_n \rightarrow 0$ as $n \rightarrow \infty$.

On the other hand, assume that for any $z = \omega^{(k,i)}(\xi_0)$ with $|\xi_0| \leq 1$, according to (3.2) the solution satisfies that

$$\left(\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0) \right) u(\xi) = g^{(k,i)}(\xi). \quad (3.5)$$

Note that method (2.6) is exact for constant function, which leads to

$$\sum_{j=0}^{k-1} w_{n,j}^{(k,i)} + \sum_{j=0}^n \omega_{n-j}^{(k,i)} = 0, \quad n \geq k,$$

and a corresponding formal power series satisfies that

$$\begin{aligned} & \sum_{n=k}^{\infty} \left(\sum_{j=0}^{k-1} w_{n,j}^{(k,i)} + \sum_{j=0}^n \omega_{n-j}^{(k,i)} \right) \xi^{n-k} \\ &= \sum_{n=0}^{\infty} \left(\sum_{j=0}^{k-1} w_{n+k,j}^{(k,i)} + \sum_{j=0}^{n+k} \omega_{n+k-j}^{(k,i)} \right) \xi^n \\ &= \sum_{n=0}^{\infty} \sum_{j=0}^{k-1} \left(w_{n+k,j}^{(k,i)} + \omega_{n+k-j}^{(k,i)} \right) \xi^n + \frac{\omega^{(k,i)}(\xi)}{1-\xi} = 0. \end{aligned}$$

Assume that $u_0 = \dots = u_{k-1} \neq 0$, then according to the expression of $g^{(k,i)}(\xi)$, it holds that $g^{(k,i)}(\xi) = u_0 \frac{\omega^{(k,i)}(\xi)}{1-\xi}$. In the case of $\omega^{(k,i)}(\xi_0) = 0$, it yields that $u(\xi) = \frac{u_0}{1-\xi}$, which means that $u_n = u_0$ for any $n \in \mathbb{N}$. And for the rest case, there is

$$u(\xi)(1-\xi) \frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0} = u_0 \frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0} + u_0 \frac{\omega^{(k,i)}(\xi_0)}{\xi - \xi_0}.$$

If assume that $u_n \rightarrow 0$ as $n \rightarrow \infty$, since according to Lemma 3.4, the coefficient sequence of $(1-\xi) \frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0}$ is in l_1 , which derives that the coefficient sequence of $u(\xi)(1-\xi) \frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0}$ tends to zero, in addition, according to Lemma 3.1, it yields that the coefficient sequence of $\frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0}$ converges to zero, however, since $\omega^{(k,i)}(\xi_0)$ and u_0 are bounded, the divergence of the coefficient sequence of $u_0 \frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0}$ for $|\xi_0| \leq 1$ leads to the contradiction. Thus, it holds that there exist some nonzero bounded initial values $\{u_i\}_{i=0}^{k-1}$ such that $u_n \not\rightarrow 0$ as $n \rightarrow \infty$, which shows that $z \notin S^{(k,i)}$. \square

According to the definition of $A(\theta)$ -stability [22] in usual case, we define the $A(\theta)$ -stability in the following sense of $0 < \alpha < 1$.

Definition 3.1. A method is said to be $A(\theta)$ -stable for $\theta \in [0, \pi - \frac{\alpha\pi}{2})$, if the sector

$$S_\theta = \{z : |\arg(-z)| \leq \theta, z \neq 0\}$$

is contained in the stability region.

Lemma 3.5. The sequence $\{s_n\}_{n=0}^\infty$ is defined by

$$s_n = \frac{1}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha} (1-s) ds, \quad n \geq 0,$$

then for $n \geq k$, there is $(-1)^k \nabla^k s_n \geq 0$.

Proof. Since for $0 \leq s \leq 1$, $0 < \alpha < 1$ and $n \geq 0$, it holds that $(n+1-s)^{-\alpha} > 0$ and $(1-s) \geq 0$, therefore $s_n \geq 0$ for any $n \geq 0$.

For $n \geq k \geq 1$, it can be verified by induction that

$$\nabla^k s_n = \frac{(-\alpha)_k}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} \left(\sum_{i=1}^k \xi_i + n - k + 1 - s \right)^{-\alpha-k} (1-s) d^k \xi ds,$$

which obtains the result. \square

Theorem 3.4. The methods (3.1) are $A(\frac{\pi}{2})$ -stable in the cases of $1 \leq i \leq k \leq 2$.

Proof. In view of the definition of $A(\theta)$ -stability, in particular, when $\theta = \frac{\pi}{2}$, it suffices to prove that $S_{\frac{\pi}{2}} \subseteq S^{(k,i)}$ for $1 \leq i \leq k \leq 2$, i.e., to prove $\omega^{(k,i)}(\xi) = 0$ for some $|\xi| \leq 1$ and $\operatorname{Re}(\omega^{(k,i)}(\xi)) > 0$ otherwise.

First of all, it can be readily checked that $\omega^{(k,i)}(1) = 0$, which implies $0 \notin S_{\frac{\pi}{2}}$. In the case of $(k, i) = (1, 1)$, resulting from the expression of $\omega^{(1,1)}(\xi)$, there is

$$\omega^{(1,1)}(\xi) = I_0 + \sum_{j=1}^{\infty} \nabla I_j \xi^j = (1-\xi)I(\xi), \quad (3.6)$$

where $I(\xi) = \sum_{n=0}^{\infty} I_n \xi^n$. Since, according to Lemma 2.1 and Theorem 3.2, we have

$$I_n = \int_0^1 r^n d\sigma(r), \quad n \in \mathbb{N}, \quad (3.7)$$

where $\sigma(r)$ is a non-decreasing function, then suppose that $|\xi| < 1$, substituting (3.7) into (3.6) yields that

$$\operatorname{Re}(\omega^{(1,1)}(\xi)) = \operatorname{Re}\left((1-\xi) \sum_{n=0}^{\infty} \int_0^1 r^n d\sigma(r) \xi^n\right) = \int_0^1 \operatorname{Re}\left(\frac{1-\xi}{1-r\xi}\right) d\sigma(r).$$

Let $\xi = |\xi|(\cos \theta + i \sin \theta)$, there is

$$\frac{1-\xi}{1-r\xi} = \frac{(1-(r+1)|\xi|\cos \theta + r|\xi|^2) + i((r-1)|\xi|\sin \theta)}{(1-r|\xi|\cos \theta)^2 + (r|\xi|\sin \theta)^2},$$

and for $0 \leq r \leq 1$ and $|\xi| < 1$, it holds that

$$\begin{aligned} 1 - (r+1)|\xi|\cos \theta + r|\xi|^2 &\geq \min((1-|\xi|\cos \theta)^2, 1-|\xi|\cos \theta), \\ 1 - 2r|\xi|\cos \theta + r^2|\xi|^2 &\leq (1+r|\xi|)^2 \leq 4, \end{aligned}$$

which arrives at

$$\int_0^1 \operatorname{Re}\left(\frac{1-\xi}{1-r\xi}\right) d\sigma(r) \geq \frac{\min((1-|\xi|\cos \theta)^2, 1-|\xi|\cos \theta)}{4} I_0.$$

In other case of $(k, i) = (2, 1)$, from the definition of $\omega^{(2,1)}(\xi)$, it induces that

$$\begin{aligned} \omega^{(2,1)}(\xi) &= \sum_{n=0}^{\infty} (\nabla I_n + \nabla^2 I_{n,1}^2) \xi^n \\ &= (1-\xi)I(\xi) + (1-\xi)^2 I_1^2(\xi) \\ &= (1-\xi)(I(\xi) - 2I_1^2(\xi) + (3-\xi)I_1^2(\xi)), \end{aligned}$$

where

$$I(\xi) = \sum_{n=0}^{\infty} I_n \xi^n, \quad I_1^2(\xi) = \sum_{n=0}^{\infty} I_{n,1}^2 \xi^n.$$

According to Lemma 3.5, Lemma 2.1 and Theorem 3.2, there exist non-decreasing functions σ and γ , respectively, such that

$$I_n - 2I_{n,1}^2 = \int_0^1 r^n d\sigma(r), \quad n = 0, 1, \dots, \quad (3.8)$$

and

$$I_{n,1}^2 = \int_0^1 r^n d\gamma(r), \quad n = 0, 1, \dots. \quad (3.9)$$

Then for $|\xi| < 1$, in place of $\omega^{(2,1)}(\xi)$, we can get

$$\operatorname{Re}\left(\omega^{(2,1)}(\xi)\right) = \int_0^1 \operatorname{Re}\left(\frac{1-\xi}{1-r\xi}\right) d\sigma(r) + \int_0^1 \operatorname{Re}\left(\frac{(1-\xi)(3-\xi)}{1-r\xi}\right) d\gamma(r).$$

Moreover, it indicates

$$\begin{aligned} \frac{(1-\xi)(3-\xi)}{1-r\xi} &= \frac{(3-4|\xi|\cos\theta + |\xi|^2\cos 2\theta)(1-r|\xi|\cos\theta) + (4-2|\xi|\cos\theta)r|\xi|^2\sin^2\theta}{(1-r|\xi|\cos\theta)^2 + (r|\xi|\sin\theta)^2} \\ &\quad + i \frac{(3r-|\xi|^2r-4+2|\xi|\cos\theta)|\xi|\sin\theta}{(1-r|\xi|\cos\theta)^2 + (r|\xi|\sin\theta)^2}, \end{aligned}$$

since

$$3-4|\xi|\cos\theta + |\xi|^2\cos 2\theta = 3-4|\xi|\cos\theta + 2|\xi|^2\cos^2\theta - |\xi|^2 \geq 2(1-|\xi|\cos\theta)^2,$$

there is

$$\int_0^1 \operatorname{Re}\left(\frac{(1-\xi)(3-\xi)}{1-r\xi}\right) d\gamma(r) \geq \frac{\min\left((1-|\xi|\cos\theta)^3, (1-|\xi|\cos\theta)^2\right)}{2} I_{0,1}^2.$$

For the rest case of $(k, i) = (2, 2)$, we begin with the equivalent form of $\omega^{(2,2)}(\xi)$, which satisfies that

$$\begin{aligned} \omega^{(2,2)}(\xi) &= I_0(1-\xi) + I_{0,1}^2(1-\xi)^2 + (1-\xi) \sum_{n=0}^{\infty} I_{n+1} \xi^n + (1-\xi)^2 \sum_{n=0}^{\infty} I_{n+1,2}^2 \xi^n \\ &= I_{0,1}^2(1-\xi)(3-\xi) + (1-\xi^2) \sum_{n=0}^{\infty} I_{n+1,1}^2 \xi^n + (1-\xi) (I(\xi) - 2I_1^2(\xi)), \end{aligned}$$

since for any $n \geq 0$, because of the relation $I_n + I_{n,2}^2 = I_{n,1}^2$, there is

$$\begin{aligned} &(1-\xi) \sum_{n=0}^{\infty} I_{n+1} \xi^n + (1-\xi)^2 \sum_{n=0}^{\infty} I_{n+1,2}^2 \xi^n \\ &= (1-\xi) \left(\sum_{n=0}^{\infty} I_{n+1,1}^2 \xi^n - \xi \sum_{n=0}^{\infty} I_{n+1,2}^2 \xi^n \right) \\ &= (1-\xi^2) \sum_{n=0}^{\infty} I_{n+1,1}^2 \xi^n + (1-\xi) \sum_{n=0}^{\infty} (I_{n+1} - 2I_{n+1,1}^2) \xi^{n+1} \\ &= (1-\xi^2) \sum_{n=0}^{\infty} I_{n+1,1}^2 \xi^n + (1-\xi) (I(\xi) - 2I_1^2(\xi) - (I_0 - 2I_{0,1}^2)). \end{aligned}$$

Consequently, suppose that $|\xi| < 1$, substituting conclusions (3.8) and (3.9) into $\omega^{(2,2)}(\xi)$, we have

$$\begin{aligned} \operatorname{Re}\left(\omega^{(2,2)}(\xi)\right) &= \int_0^1 \operatorname{Re}\left((1-\xi)(3-\xi)\right) d\gamma(r) \\ &\quad + \int_0^1 r \operatorname{Re}\left(\frac{1-\xi^2}{1-r\xi}\right) d\gamma(r) + \int_0^1 \operatorname{Re}\left(\frac{1-\xi}{1-r\xi}\right) d\sigma(r), \end{aligned}$$

furthermore, there is

$$\begin{aligned} \frac{1 - \xi^2}{1 - r\xi} &= \frac{(1 - |\xi|^2 \cos 2\theta)(1 - r|\xi| \cos \theta) + r|\xi|^3 \sin \theta \sin 2\theta}{(1 - r|\xi| \cos \theta)^2 + (r|\xi| \sin \theta)^2} \\ &\quad + i \frac{(1 - |\xi|^2 \cos 2\theta)r|\xi| \sin \theta - (1 - r|\xi| \cos \theta)r^2 \sin 2\theta}{(1 - r|\xi| \cos \theta)^2 + (r|\xi| \sin \theta)^2}. \end{aligned}$$

Since for $0 \leq r \leq 1$, it holds that

$$\begin{aligned} &(1 - |\xi|^2 \cos 2\theta)(1 - r|\xi| \cos \theta) + r|\xi|^3 \sin \theta \sin 2\theta \\ &= 1 - |\xi|^2 \cos 2\theta - r|\xi| \cos \theta + r|\xi|^3 \cos \theta \\ &\geq (1 - |\xi|^2)(1 - |\xi| |\cos \theta|), \end{aligned}$$

then, we may see that

$$\int_0^1 r \operatorname{Re} \left(\frac{1 - \xi^2}{1 - r\xi} \right) d\gamma(r) \geq \frac{(1 - |\xi|^2)(1 - |\xi| |\cos \theta|)}{4} \int_0^1 r d\gamma(r) = \frac{(1 - |\xi|^2)(1 - |\xi| |\cos \theta|)}{4} I_{1,1}^2.$$

As a result, for $1 \leq i \leq k \leq 2$, it demonstrates that

$$\operatorname{Re} \left(\omega^{(k,i)}(\xi) \right) \geq \frac{\min((1 - |\xi| \cos \theta)^2, 1 - |\xi| \cos \theta)}{4} I_0 > 0, \quad |\xi| < 1.$$

In addition, for any fixed ξ lying on the unit circle, the angle of which satisfying $\arg(\xi) = \theta_\xi \neq 0$, correspondingly, there exists a sequence $\xi_n = (1 - \frac{1}{n})\xi$ with $|\xi_n| < 1$ for any $n = 1, 2, \dots$, then according to Lemma 3.4, there exists constant $M^{(k,i)} > 0$ such that

$$|\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)| \leq \frac{M^{(k,i)}}{|1 - \xi|} |\xi - \xi_0|, \quad \xi \neq 1,$$

which yields the pointwise continuity of $\omega^{(k,i)}(\xi)$ for $|\xi| \leq 1$ with the exception of $\xi = 1$. Therefore it holds that

$$\operatorname{Re} \left(\omega^{(k,i)}(\xi) \right) = \lim_{n \rightarrow \infty} \operatorname{Re} \left(\omega^{(k,i)}(\xi_n) \right) \geq \frac{I_0}{4} \min((1 - \cos \theta_\xi)^2, 1 - \cos \theta_\xi) > 0.$$

□

4 Numerical experiments

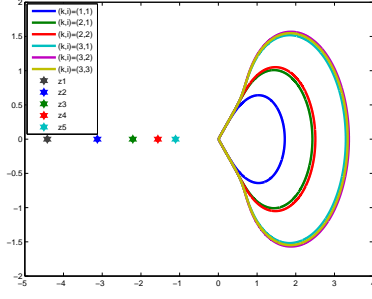
Example 4.1. We consider the linear equation

$$\begin{cases} {}^C D^\alpha u(t) = \lambda u(t) + f(t), & t \in (0, 1], \\ u(0) = u_0 \end{cases} \quad (4.1)$$

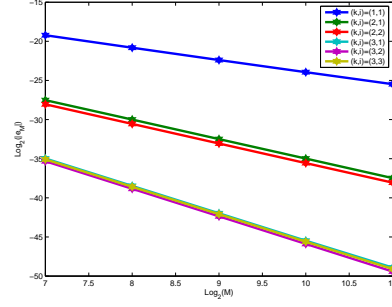
with $0 < \alpha < 1$. The exact solution is $u(t) = e^{-t}$ and $f(t) = -t^{1-\alpha} E_{1,2-\alpha}(-t) - \lambda e^{-t}$, where the Mittag-Leffler function [39] is defined by

$$E_{\alpha,\beta}(t) = \sum_{k=0}^{\infty} \frac{t^k}{\Gamma(\alpha k + \beta)}, \quad \alpha > 0, \beta > 0.$$

Figures 1(a), 2(a) and 3(a) show the truncated curves $\sum_{n=0}^{6000} \omega_n^{(k,i)} e^{in\theta}$ for various α in the examples of $1 \leq i \leq k \leq 3$. It is known from Theorem 3.3 that the stability regions of methods (3.1) are outside the corresponding curves. Figures 1(b), 2(b) and 3(b) list the global error e_M of Example 4.1 on the logarithm scale, where e_n is the difference between the exact solution of (4.1) and the computed solution at the time step $n\Delta t$ with $\Delta t = 1/M$, $M = 2^j$, $7 \leq j \leq 11$.

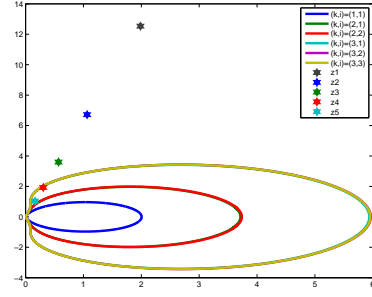


(a) boundary of numerical stability region

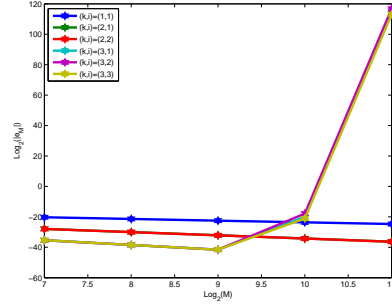


(b) error and convergence order

Figure 1: $\alpha = 0.5, \lambda = -50$



(a) boundary of numerical stability region



(b) error and convergence order

Figure 2: $\alpha = 0.9, \lambda = 1000 \times e^{\frac{i\pi\alpha}{2}}$

In Figure 1, we can observe that the points $z_n := \lambda(\Delta t_n)^\alpha$ ($1 \leq n \leq 5$) fall into the stability regions, in which situation e_M obtains the reliable accuracy and predicted convergence order of $O(\Delta t^{k+1-\alpha})$.

In Figure 2, choosing points $\{z_n\}_{n=1}^5$ on the half line with angle $\frac{\pi\alpha}{2}$, according to Figure 2(a), we may see that when all $\{z_n\}_{n=1}^5$ fall into the stability regions for $k = 1, 2$, correspondingly, as shown in Figure 2(b), the error e_M agrees with the expectation of order accuracy. For $k = 3$, due to z_4, z_5 outside the stability regions, the errors arising from numerical discretisation and the round-off error will be accumulated significantly.

In Figure 3, for imaginary number λ , according to Theorem 3.4, every point z belongs to the stability domains of methods (3.1) in the cases of $k = 1, 2$, and the error accuracy and convergence order in Figure 3(b) confirm the theoretical result. As a counter example, when z_3 doesn't belong to the stability region for $\alpha = 0.98$ in Figure 3(a), the corresponding error e_M shown in Figure 3(b) can't ensure the desirable result. In fact, it can be observed that for $k = 3$ methods (3.1) are not $A(\frac{\pi}{2})$ -stable for some α closed to 1.

Example 4.2. Consider the nonlinear equation

$$\begin{cases} {}^C D^\alpha u(t) = -u^2 + f(t), & t \in (0, 1] \\ u(0) = u_0 \end{cases} \quad (4.2)$$

with exact solution $u(t) = e^{\mu t}$ and source function $f(t) = \mu t^{1-\alpha} E_{1,2-\alpha}(\mu t) + e^{2\mu t}$.

Figure 4 and 5 plot the global error e_M on logarithm scale in Example 4.2 for different μ and α , where $\Delta t = 1/M$, $M = 2^j$, $2 \leq j \leq 11$. It is observed that the theoretical convergence rate is confirmed in the examples with $1 \leq i \leq k \leq 3$ when using discretisation formula (2.6) in combination with Newton's method for the nonlinear equation behind the implicit method.

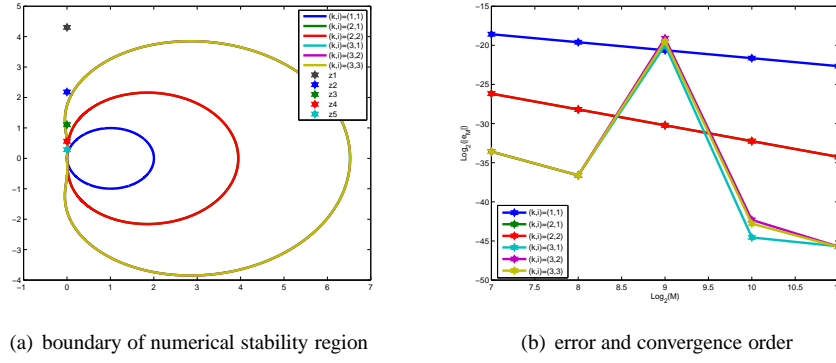


Figure 3: $\alpha = 0.98$, $\lambda = 500i$

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References

- [1] L. Aceto, C. Magherini, and P. Novati. Fractional convolution quadrature based on generalized Adams methods. *Calcolo*, 51:441–463, 2014.
- [2] L. Aceto, C. Magherini, and P. Novati. On the construction and properties of m -step methods for FDEs. *SIAM Journal on Scientific Computing*, 37(2):653–675, 2015.
- [3] N. I. Akhiezer. *The Classical Moment Problem*. Oliver & Body, 1965.
- [4] A. A. Alikhanov. A new difference scheme for the time fractional diffusion equation. *Journal of Computational Physics*, 280:424–438, Jan 2015.
- [5] R. Bagley and P. Torvik. A theoretical basis for the application of fractional calculus to viscoelasticity. *Journal of Rheology*, 27(3):201–210, 183.
- [6] D. Baleanu, K. Diethelm, E. Scalas, and J. Trujillo. *Fractional calculus, models and numerical methods*, volume 3 of *Series on Complexity, Nonlinearity and Chaos*. World Scientific, 2011.
- [7] E. Barkai, R. Metzler, and J. Klafter. From continuous time random walks to the fractional Fokker-Planck equation. *PHYSICAL REVIEW E*, 61(1):132–138, 2000.
- [8] D. Benson, S. Wheatcraft, and M. Meerschaert. Application of a fractional advection-dispersion equation. *Water Resources Research*, 36(6):1403–1412, 2000.
- [9] H. Brunner and P. J. van der Houwen. *The numerical solution of Volterra equations*, volume 3 of *CWI monograph*. Elsevier Science Publishers B.V., 1986.
- [10] M. Caputo. *Elasticità e Dissipazione*. Zanichelli, Bologna, 1969.
- [11] A. Carpinteri and F. Mainardi, editors. *Fractals and Fractional Calculus in Continuum Mechanics*. Springer, 1997.
- [12] K. Diethelm. A predictor-corrector approach for the numerical solution of fractional differential equations. *Nonlinear Dynamics*, 29(1-4):3–22, 2002.
- [13] K. Diethelm. *The Analysis of Fractional Differential Equations*. Lecture Notes in Mathematics. Springer, 2004.

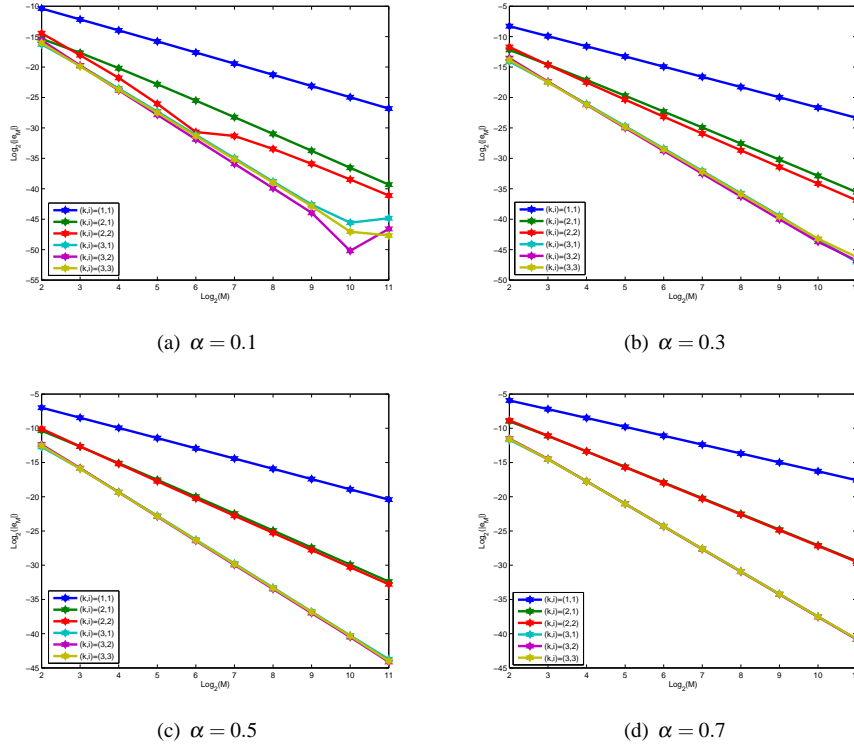


Figure 4: error and convergence order for $\mu = -1$

- [14] K. Diethelm. An investigation of some nonclassical methods for the numerical approximation of Caputo-type fractional derivatives. *Numerical Algorithms*, 47(4):361–390, 2008.
- [15] K. Diethelm, N. Ford, A. Freed, and Y. Luchko. Algorithms for the fractional calculus: a selection of numerical methods. 194:743–773, 2005.
- [16] K. Diethelm and G. Waltz. Numerical solution of fractional order differential equations by extrapolation. *Numerical Algorithms*, 16:231–253, 1997.
- [17] A. Erdelyi. On fractional integration and its applications to the theory of Hankel transforms. *Quarterly Journal of Mathematics*, 11:293–303, 1940.
- [18] N. Ford and A. Simpson. The numerical solution of fractional differential equations: speed versus accuracy. *Numerical Algorithms*, 26(4):333–346, 2001.
- [19] G. Gao, Z. Z. Sun, and H. W. Zhang. A new fractional numerical differentiation formula to approximate the caputo fractional derivative and its applications. *Journal of Computational Physics*, 259:33–50, 2014.
- [20] R. Garappa. A family of Adams exponential integrators for fractional linear systems. *Computers & Mathematics with Applications*, 66(5):717–727, 2013.
- [21] R. Garappa and M. Popolizio. Generalized exponential time differencing methods for fractional order problems. *Computers & Mathematics with Applications*, 62(3):876–890, 2011.
- [22] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*, volume 14 of *Springer Series in Computational Mathematics*. Springer, 1991.
- [23] E. Hairer, G. Wanner, and S. P. Norsett. *Solving Ordinary Differential Equations I: Nonstiff Problems*, volume 8 of *Springer Series in Computational Mathematics*. Springer, 1987.
- [24] R. Herrmann. *Fractional Calculus, an Introduction for Physicists*. World Scientific, 2014.

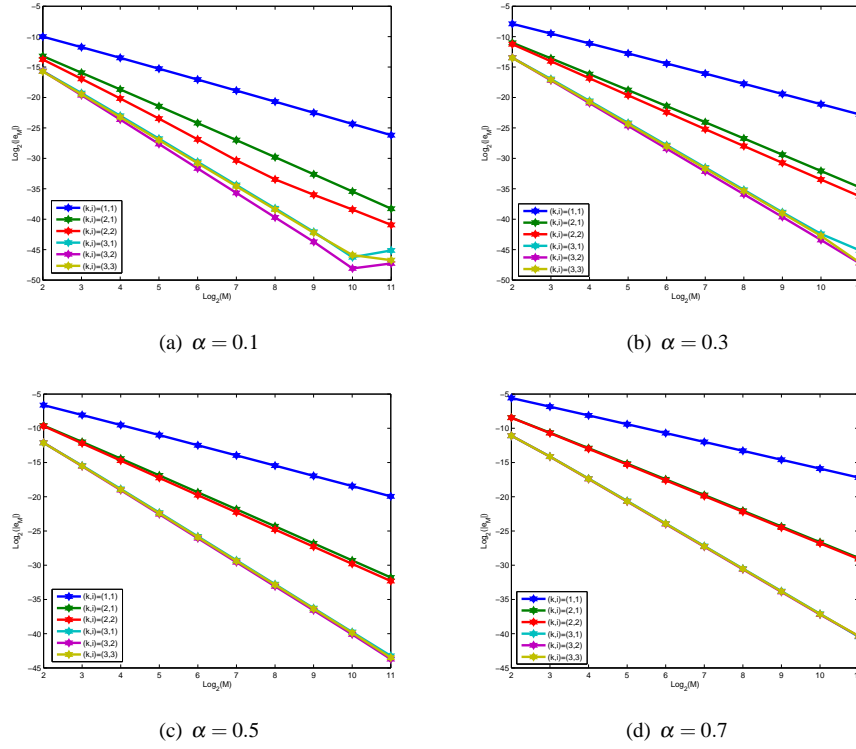


Figure 5: error and convergence order for $\mu = i$

- [25] R. Hilfer, editor. *Applications of fractional calculus in physics*. World Scientific, 2000.
- [26] A. Kilbas, H. Srivastava, and J. Trujillo. *Theory and applications of fractional differential equations*, volume 204 of *North-Holland Mathematics Studies*. Elsevier, 2006.
- [27] T. Langlelands, B. Henry, and S. Wearne. Fractional cable equation models for anomalous electrodiffusion in nerve cells: infinite domain solutions. *Journal of Mathematical Biology*, 59:761–808, 2009.
- [28] C. Li and F. Zeng. *Numerical methods for fractional calculus*. CRC Press, Taylor & Francis Group, 2015.
- [29] Y. M. Lin and C. J. Xu. Finite difference/spectral approximations for the time-fractional diffusion equation. *Journal of Computational Physics*, 225(2):1533–1552, 2007.
- [30] F. Liu, V. Anh, I. Turner, and P. Zhuang. Time fractional advection-dispersion equation. *Journal of Applied Mathematics and Computing*, 13:233–245, 2003.
- [31] C. Lubich. On the stability of linear multistep methods for Volterra convolution equations. *IMA Journal of Numerical Analysis*, 3:439–465, 1983.
- [32] C. Lubich. Discretized fractional calculus. *SIAM Journal on Mathematical Analysis*, 17(3):704–719, 1986.
- [33] C. Lubich. A stability analysis of convolution quadratures for Abel-Volterra integral equations. *IMA Journal of Numerical Analysis*, 6(6):87–101, 1986.
- [34] C. Lubich. Convolution quadrature and discretized operational calculus. I. *Numerische Mathematik*, 52(2):129–146, 1988.
- [35] D. Matignon. Stability results for fractional differential equations with applications to control processing. In *Computational Engineering in Systems Applications*, pages 963–968, 1996.

- [36] R. Metzler and J. Klafter. The random walk's guide to anomalous diffusion: a fractional dynamics approach. *Physics Reports*, 339(1):1–77, 2000.
- [37] K. Miller and B. Ross. *An Introduction to Fractional Calculus and Fractional Differential Equations*. Wiley, New York, 1993.
- [38] K. Oldham and J. Spanier. *The Fractional Calculus*. Academic Press, New York, 1974.
- [39] I. Podlubny. *Fractional Differential Equations*. Academic Press, San Diego, 1999.
- [40] W. Rudin. *Real and Complex Analysis*. McGraw-Hill, 1987.
- [41] S. Samko, A. Kilbas, and O. Marichev. *Fractional Integrals and Derivatives*. Gordon and Breach Science Publishers, 1993.
- [42] F. Santamaria, S. Wils, E. de Schutter, and G. Augustine. Anomalous diffusion in Purkinje cell dendrites caused by spines. *Neuron*, 52:635–648, 2006.
- [43] E. Scalas, R. Gorenflo, and F. Mainardi. Fractional calculus and continuous-time finance. *Physica A: Statistical Mechanics and its Applications*, 284(1-4):376–384, 2000.
- [44] J. A. Shohat and J. D. Tamarkin. *The problem of Moments*, volume 1 of *Mathematical Surveys and Monographs*. American Mathematical Society, fourth edition, 1970.
- [45] W. Wyss. The Fractional Black-Scholes equation. *Fractional Calculus & Applied Analysis*, 3:51–61, 2000.
- [46] A. Zygmund. *Trigonometric series*, volume 1. Cambridge university press, 2002.